

Synthesis of new N-acylantipyrylureas and the crystal structure of N-benzoyl-N'-[4-(2,3-dimethyl-1-phenylpyrazol-5-one)]urea

Fedotova N., Litvinov I., Kataeva O.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

New derivatives of acylheterylureas were synthesized by reactions of acylisocyanates with 4-amino-2,3-dimethyl-1-phenylpyrazol-5-one. The structures of the compounds obtained have been established by IR and ¹H NMR spectroscopy. N-Benzoyl-N'-[4-(1-phenyl-2,3-dimethylpyrazol-5-one)]urea has been studied by X-ray structural analysis. It was found that the molecule adopts an anti-syn conformation stabilized by an intramolecular hydrogen bond. In the crystal, molecules are linked in centrosymmetric dimers via intermolecular hydrogen bonds. © 1996 Plenum Publishing Corporation.

Keywords

2,3-dimethyl-1-phenylpyrazol-5-one, Acylisocyanates, Biological activity, Hydrogen bonds, N-benzoyl-N'-[4-(2,3-dimethyl-1-phenylpyrazol-5-one)]urea, X-ray structural study